

On the ground state energy scaling in quasi-rung-dimerized spin ladders

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On the basis of periodic boundary conditions we study perturbatively a large N asymptotics (N is the number of rungs) for the ground state energy density and gas parameter of a spin ladder with slightly destroyed rung-dimerization. Exactly rung-dimerized spin ladder is treated as the reference model. Explicit perturbative formulas are obtained for three special classes of spin ladders.

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I. INTRODUCTION

Phase structure of frustrated spin ladders and spin ladders with four-spin terms has been intensively studied in the last decade both theoretically and numerically^{1–3}. Among other phases the mathematically most simple one and at the same time, probably, the one most interesting for physical applications is the so called rung-singlet (or rung-dimerized) phase^{4,5}. Within it the ground state may be well approximated by an infinite tensor product of rung-dimers (singlet pairs)

$$|0\rangle_{r-d} = \otimes_n |0\rangle_n. \quad (1)$$

This state will be an *exact* ground state only for rather big antiferromagnetic rung-coupling and under a special condition on the coupling constants⁴. The latter has no physical background and thus there are absolutely no grounds to assume its relevance for real compounds. Nevertheless it is a common opinion that for rather big antiferromagnetic rung coupling a spin ladder should still remain in the rung-singlet phase. This means that all physical properties of such a ladder may be obtained perturbatively on the basis of the "bare" ground state (1) and its excitations. Together with verification by machinery calculations this approach should give a comprehensive description of the rung-singlet phase. A machinery calculation will provide excellent tests for suggested formulas while a perturbative formula will give a right direction for numerical research and interpretation of the obtained data.

Such approach has two main difficulties. First of all a general spin ladder model is non-integrable and although one- and two-magnon states may be readily derived within Bethe Ansatz, three-magnon states are obtained now only for five special integrable models^{6,7}. The second difficulty originates from the fact that an analytical result is usually obtained for infinite ladder however in a numerical calculation a ladder has a finite size. Hence in order to use a machinery calculation for verification of an analytical result one has to perform a correct extrapolation of the numerical data. This means that utilizing a finite number of numerical estimations f_N of some value f (N the number rungs of the ladder) it is necessary to estimate the limit $f_\infty = \lim_{N \rightarrow \infty} f_N$. On this way, in addition to a number of sequence transformation meth-

ods improving the convergence⁸, one has to be guided by some extrapolation formula. The latter may be guessed by an analysis of numerical data⁹, or suggested theoretically on the basis of conformal field theory¹⁰ predictions, or on some other argumentation¹¹.

Taking an exact rung-dimerized spin ladder as a reference model, it is natural to treat the ground state of a spin ladder with violated rung-dimerization as a dilute magnon gas¹². Its concentration (gas parameter)

$$\rho \equiv \rho_\infty = \lim_{N \rightarrow \infty} \rho_N, \quad \rho_N = \frac{\langle 0 | \hat{Q} | 0 \rangle}{N}, \quad (2)$$

(\hat{Q} is a magnon number operator (13)) and energy density

$$E \equiv E_\infty = \lim_{N \rightarrow \infty} E_N, \quad E_N = \frac{\langle 0 | \hat{H} | 0 \rangle}{N}, \quad (3)$$

turns to zero for an exact rung-dimerized spin ladder and hence they should be good governing parameters for a perturbation theory based on the gas approximation. Perturbative expressions for ρ and E were derived in Ref. 12. In the present paper assuming *periodic* boundary conditions we obtain in three special cases the corresponding extrapolation formulas for ρ_N and E_N .

The two formulas

$$E_N = E_\infty + (-1)^N A \frac{e^{-N/N_0}}{N^2}, \quad (4)$$

$$E_N = E_\infty - \frac{A}{N^2}, \quad (5)$$

(A and N_0 are free parameters) have already been suggested correspondingly for open^{13,14} and periodic¹⁰ boundary conditions. The expression (4) was implied ad hoc, while Eq. (5) follows from conformal theory argumentation. The perturbative formulas obtained below for three special classes of spin ladders have a rather different form

$$E_N = E_\infty + (A + (-1)^N B) e^{-(N-1)/N_0}. \quad (6)$$

II. DESCRIPTION OF THE MODEL

We shall use an equivalent representation^{6,12}

$$\hat{H} = \hat{H}_0 + J_6 \hat{V}, \quad (7)$$

of the spin ladder Hamiltonian¹⁻⁵. Here J_6 is a perturbation parameter and

$$\begin{aligned}\hat{H}_0 &= \sum_{n=1}^N J_1 Q_n + J_2 (\Psi_n \cdot \bar{\Psi}_{n+1} + \bar{\Psi}_n \cdot \Psi_{n+1}) \\ &\quad + J_3 Q_n Q_{n+1} + J_4 \mathbf{S}_n \cdot \mathbf{S}_{n+1} + J_5 (\mathbf{S}_n \cdot \mathbf{S}_{n+1})^2, \\ \hat{V} &= \sum_{n=1}^N V_{n,n+1},\end{aligned}\quad (8)$$

$$\begin{aligned}\mathbf{S}_n &= \mathbf{S}_{1,n} + \mathbf{S}_{2,n}, \quad Q_n = \frac{1}{2} \mathbf{S}_n^2, \\ V_{n,n+1} &= \bar{\Psi}_n \cdot \bar{\Psi}_{n+1} + \Psi_n \cdot \Psi_{n+1},\end{aligned}\quad (9)$$

($\mathbf{S}_{i,n}$ for $i = 1, 2$ are spin-1/2 operators associated with n -th rung). The local operators

$$\begin{aligned}\Psi_n &= \frac{1}{2} (\mathbf{S}_{1,n} - \mathbf{S}_{2,n}) - i [\mathbf{S}_{1,n} \times \mathbf{S}_{2,n}], \\ \bar{\Psi}_n &= \frac{1}{2} (\mathbf{S}_{1,n} - \mathbf{S}_{2,n}) + i [\mathbf{S}_{1,n} \times \mathbf{S}_{2,n}],\end{aligned}\quad (10)$$

may be interpreted as (neither Bose nor Fermi) creation-annihilation operators for rung-triplets. Namely

$$\begin{aligned}\bar{\Psi}_n^a |0\rangle_n &= |1\rangle_n^a, & \bar{\Psi}_n^a |1\rangle_n^b &= 0, \\ \Psi_n^a |0\rangle_n &= 0, & \Psi_n^a |1\rangle_n^b &= \delta_{ab} |0\rangle_n.\end{aligned}\quad (11)$$

From (8) and (9) readily follows⁶ that

$$[\hat{H}_0, \hat{Q}] = 0, \quad (12)$$

where the operator

$$\hat{Q} = \sum_n Q_n, \quad (13)$$

according to relations

$$Q_n |0\rangle = 0, \quad Q_m |1\rangle_n = \delta_{mn} |1\rangle_n, \quad (14)$$

has a sense of the number operator for rung-triplets⁶.

For rather big J_1 (for example necessary should be^{4,6} $J_1 > J_2$) vector (1) is the *zero energy* ($\hat{H}_0 |0\rangle_{r-d} = 0$) ground state for \hat{H}_0 , whose physical Hilbert space splits into a direct sum^{4,6,12}

$$\mathcal{H} = \sum_{m=0}^{\infty} \mathcal{H}^m, \quad \hat{Q}|_{\mathcal{H}^m} = m. \quad (15)$$

The subspace \mathcal{H}^0 is generated by the single vector (1). According to (2), (3) and (8)

$$\rho_N = \frac{\partial E_N}{\partial J_1}. \quad (16)$$

Since $\hat{V} : |0\rangle_{r-d} \rightarrow \mathcal{H}^2$, a perturbative treatment of the term $J_6 \hat{V}$ gives

$$E_N = -\frac{J_6^2}{N} \sum_{|\mu\rangle \in \mathcal{H}^2} \frac{|\langle \mu | \hat{V} | 0 \rangle_{r-d}|^2}{E(\mu)} + o(J_6^2), \quad (17)$$

where all the states $|\mu\rangle$ in the sum have zero total spin and quasimomentum. In the $N \rightarrow \infty$ limit¹²

$$\begin{aligned}E_\infty &= -\Theta(\Delta_0^2 - 1) \frac{3J_6^2(\Delta_0^2 - 1)}{\Delta_0^2 E_{bound}} \\ &\quad - \frac{3J_6^2}{4J_2 \Delta_0} \left(1 - \frac{J_2 |\Delta_0^2 - 1| + 2\Delta_0 \sqrt{J_1^2 - J_2^2}}{[2\Delta_0 J_1 + (\Delta_0^2 + 1)J_2]} \right),\end{aligned}\quad (18)$$

where $\Theta(x) = 1$ for $x > 0$ and $\Theta(x) = 0$ for $x \leq 0$ and

$$\Delta_0 = \frac{J_3 - 2J_4 + 4J_5}{2J_2}, \quad (19)$$

$$E_{bound} = 4J_1 + 2J_2 \left(\Delta_0 + \frac{1}{\Delta_0} \right). \quad (20)$$

III. A FINITE- N TWO-PARTICLE PROBLEM

A zero total spin and quasimomentum two-magnon state has the following general form,

$$|2 - magn\rangle = \sum_{1 \leq m < n \leq N} a(n-m) \dots |1\rangle_m^a \dots |1\rangle_n^a \dots \quad (21)$$

The dimension of the corresponding Hilbert space is $N/2$ for even N and $(N-1)/2$ for odd. The wave function $a(n)$ should be normalised

$$\sum_{n=1}^{N-1} (N-n) |a(n)|^2 = \sum_{m < n} |a(n-m)|^2 = \frac{1}{3}, \quad (22)$$

and satisfy the periodicity condition $a(n-m) = a(m+N-n)$ or shortly

$$a(n) = a(N-n). \quad (23)$$

Performing a substitution $n \rightarrow N-n$ and using (23) one can obtain from (22)

$$\sum_{n=1}^{N-1} n |a(N-n)|^2 = \sum_{n=1}^{N-1} n |a(n)|^2 = \frac{1}{3}. \quad (24)$$

Together (22) and (24) result in

$$\sum_{n=1}^{N-1} |a(n)|^2 = \frac{2}{3N}. \quad (25)$$

The Schrödinger equation gives

$$4J_1 a(n) + 2J_2 [a(n-1) + a(n+1)] = E a(n) \quad (26)$$

for $1 < n < N-1$ and

$$2(2J_1 + J_2 \Delta_0) a(1) + 2J_2 a(2) = E a(1), \quad (27)$$

for $n = 1$.

General solution of the system (26), (27) has the form

$$a(n, z) = \frac{1}{\sqrt{Z(z)}} \left[\left(1 - \frac{\Delta_0}{z}\right) z^n - \frac{1}{z^n} \left(1 - \Delta_0 z\right) \right], \quad (28)$$

and dispersion

$$E(z) = 4J_1 + 2J_2 \left(z + \frac{1}{z} \right). \quad (29)$$

The normalization constant $Z(z)$ ensures condition (25). The parameter z corresponds to relative quasimomentum of magnon pair and satisfy an equation

$$z^{N-1} = \frac{\Delta_0 z - 1}{z - \Delta_0} = -z \frac{\Delta_0 - 1/z}{\Delta_0 - z}. \quad (30)$$

The latter is invariant under complex conjugation and a duality symmetry

$$z \rightarrow \frac{1}{z}, \quad (31)$$

which according to (28) is related to multiplication of the wave function on (-1) . Hence for even N the roots of (30) are joined in dual pairs, while for odd N there is an additional autodual root $z = -1$.

In the three special cases $\Delta_0 = -1$, $\Delta_0 = 1$ and $\Delta_0 = 0$ Eq. (30) may be solved explicitly. Denoting the corresponding solutions as u_j , v_j and w_j respectively one has

$$\begin{aligned} u_j &= e^{(2j+1)i\pi/(N-1)}, \quad j = 0, \dots, N-2, \quad (\Delta_0 = -1), \\ v_j &= e^{2ji\pi/(N-1)}, \quad j = 0, \dots, N-2, \quad (\Delta_0 = 1), \\ w_j &= e^{(2j+1)i\pi/N}, \quad j = 0, \dots, N-1, \quad (\Delta_0 = 0). \end{aligned} \quad (32)$$

Taking into account that all the roots (32) lie in a unite circle one may readily get

$$\begin{aligned} Z(z) &= 3N(N-1)(1 - \Delta_0 z) \left(1 - \frac{\Delta_0}{z}\right), \quad \Delta_0 = \pm 1, \\ Z(z) &= 3N^2, \quad \Delta_0 = 0, \end{aligned} \quad (33)$$

and then

$$\begin{aligned} |a(n, z)|^2 &= \frac{1}{3N(N-1)} \left[2 + \Delta_0 \left(z^{2n-1} + \frac{1}{z^{2n-1}} \right) \right], \\ \Delta_0 &= \pm 1, \\ |a(n, z)|^2 &= \frac{1}{3N^2} \left(2 - z^{2n} - \frac{1}{z^{2n}} \right), \quad \Delta_0 = 0. \end{aligned} \quad (34)$$

IV. EXACT RESULTS AT $\Delta_0 = 0$ AND $\Delta_0 = \pm 1$

Let $|z\rangle$ be the state related to wave function (28). From (9) and (21) follows that

$$|\langle z | \hat{V} | 0 \rangle_{r-d}|^2 = 9N^2 |a(1, z)|^2. \quad (35)$$

For the evaluation of E_N one has to perform in (17) a summation over all duality pairs of roots. Since both the roots in a pair give the same contribution this is equivalent to inserting the factor $1/2$ before summation over *all* roots. Hence (17) and (35) result in

$$E_N(\Delta_0) = -\frac{3}{4} J_6^2 G_N(\Delta_0) + o(J_6^2), \quad (36)$$

where

$$\begin{aligned} G_N(-1) &= \frac{1}{N-1} \sum_{j=0}^{N-2} \frac{2 - (u_j + 1/u_j)}{2J_1 + J_2(u_j + 1/u_j)} = \frac{1}{J_2(N-1)} \sum_{j=0}^{N-2} \left[-1 + \frac{J_1 + J_2}{\sqrt{J_1^2 - J_2^2}} \left(\frac{J_-}{J_- - u_j} - \frac{J_+}{J_+ - u_j} \right) \right], \\ &= \frac{1}{J_2} \left[\frac{J_1 + J_2}{\sqrt{J_1^2 - J_2^2}} \left(\frac{J_-^{N-1}}{J_-^{N-1} + 1} - \frac{J_+^{N-1}}{J_+^{N-1} + 1} \right) - 1 \right], \\ G_N(1) &= \frac{1}{N-1} \sum_{j=0}^{N-2} \frac{2 + (v_j + 1/v_j)}{2J_1 + J_2(v_j + 1/v_j)} = \frac{1}{J_2(N-1)} \sum_{j=0}^{N-2} \left[1 - \frac{J_1 - J_2}{\sqrt{J_1^2 - J_2^2}} \left(\frac{J_-}{J_- - v_j} - \frac{J_+}{J_+ - v_j} \right) \right], \\ &= \frac{1}{J_2} \left[1 - \frac{J_1 - J_2}{\sqrt{J_1^2 - J_2^2}} \left(\frac{J_-^{N-1}}{J_-^{N-1} + (-1)^{N-1}} - \frac{J_+^{N-1}}{J_+^{N-1} + (-1)^{N-1}} \right) \right], \\ G_N(0) &= \frac{1}{N} \sum_{j=0}^{N-1} \frac{2w_j^2 - w_j^4 - 1}{w_j(J_2w_j^2 - 2J_1w_j + J_2)} = \frac{2}{J_2^2 N} \sum_{j=0}^{N-1} \left[J_1 - \frac{J_2}{2} \left(w_j + \frac{1}{w_j} \right) - \sqrt{J_1^2 - J_2^2} \left(\frac{J_-}{J_- - w_j} - \frac{J_+}{J_+ - w_j} \right) \right] \\ &= 2 \left[\frac{J_1}{J_2^2} - \frac{\sqrt{J_1^2 - J_2^2}}{J_2^2} \left(\frac{J_-^N}{J_-^N + 1} - \frac{J_+^N}{J_+^N + 1} \right) \right], \end{aligned} \quad (37)$$

and

$$J_{\pm} = \frac{-J_1 \pm \sqrt{J_1^2 - J_2^2}}{J_2}. \quad (38)$$

In (37) we used for calculations the formulas

$$\begin{aligned} \sum_{j=0}^{N-2} \frac{1}{J - u_j} &= \frac{(N-1)J^{N-2}}{J^{N-1} + 1}, \\ \sum_{j=0}^{N-2} \frac{1}{J - v_j} &= \frac{(N-1)J^{N-2}}{J^{N-1} + (-1)^{N-1}}, \end{aligned}$$

which may be proved according to the following argumentation. The sums in (39) are fractions whose numerator and denominator are symmetric polynomials with respect to u_j , v_j and w_j respectively. However according to (30) all these polynomials except

$$\begin{aligned} u_0 \dots u_{N-2} &= (-1)^{N-1}, & v_0 \dots v_{N-2} &= 1, \\ w_0 \dots w_{N-1} &= (-1)^N \end{aligned} \quad (40)$$

are equal to zero.

From equality $J_+ J_- = 1$ readily follows

$$\begin{aligned} \frac{J_-^{N-1}}{J_-^{N-1} + 1} - \frac{J_+^{N-1}}{J_+^{N-1} + 1} &= \frac{1 - J_+^{N-1}}{1 + J_+^{N-1}}, \\ \frac{J_-^{N-1}}{J_-^{N-1} + (-1)^{N-1}} - \frac{J_+^{N-1}}{J_+^{N-1} + (-1)^{N-1}} &= \frac{1 - (-J_+)^{N-1}}{1 + (-J_+)^{N-1}}. \end{aligned} \quad (41)$$

Using (41) one may readily reduce Eqs. (37) to the form

$$\begin{aligned} G_N(-1) &= \frac{1}{J_2} \left[\sqrt{\frac{J_1 + J_2}{J_1 - J_2}} \cdot \frac{1 - J_+^{N-1}}{1 + J_+^{N-1}} - 1 \right], \\ G_N(1) &= \frac{1}{J_2} \left[1 - \sqrt{\frac{J_1 - J_2}{J_1 + J_2}} \cdot \frac{1 - (-J_+)^{N-1}}{1 + (-J_+)^{N-1}} \right], \\ G_N(0) &= \frac{2}{J_2} \left[\frac{J_1}{J_2} - \frac{\sqrt{J_1^2 - J_2^2}}{J_2} \cdot \frac{1 - J_+^N}{1 + J_+^N} \right]. \end{aligned} \quad (42)$$

It may be readily observed that the corresponding values for $E_\infty(\Delta_0)$ agree with Eq. (18). The scaling law has the form (6) with

$$\begin{aligned} A(-1) &= 0, & B(-1) &= -\frac{3J_6^2}{2J_2} \sqrt{\frac{J_1 + J_2}{J_1 - J_2}}, \\ A(1) &= \frac{3J_6^2}{2J_2} \sqrt{\frac{J_1 - J_2}{J_1 + J_2}}, & B(1) &= 0, \\ A(0) &= 0, & B(0) &= \frac{3J_6^2}{J_2^2} \sqrt{J_1^2 - J_2^2}, \end{aligned} \quad (43)$$

at $J_2 > 0$ and

$$\begin{aligned} A(-1) &= -\frac{3J_6^2}{2J_2} \sqrt{\frac{J_1 + J_2}{J_1 - J_2}}, & B(-1) &= 0, \\ A(1) &= 0, & B(1) &= -\frac{3J_6^2}{2J_2} \sqrt{\frac{J_1 - J_2}{J_1 + J_2}}, \\ A(0) &= \frac{3J_6^2}{J_2^2} \sqrt{J_1^2 - J_2^2}, & B(0) &= 0, \end{aligned} \quad (44)$$

at $J_2 < 0$. In both the cases

$$N_0 = \frac{1}{\ln |J_2| - \ln (J_1 - \sqrt{J_1^2 - J_2^2})}. \quad (45)$$

The corresponding formulas for ρ_N have the similar form and may be readily obtained from (16).

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